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DOI: <https://doi.org/10.1103/PhysRevD.91.114012>

Posted at the Zurich Open Repository and Archive, University of Zurich

ZORA URL: <https://doi.org/10.5167/uzh-121357>

Journal Article

Accepted Version

Originally published at:

Beaujean, Frederik; Chrzęszcz, Marcin; Serra, Nicola; van Dyk, Danny (2015). Extracting angular observables without a likelihood and applications to rare decays. *Physical Review D (Particles, Fields, Gravitation and Cosmology)*, 91:114012.

DOI: <https://doi.org/10.1103/PhysRevD.91.114012>

Extracting Angular Observables without a Likelihood and Applications to Rare Decays

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Our goal is to obtain a complete set of angular observables arising in a generic multi-body process. We show how this can be achieved without the need to carry out a likelihood fit of the angular distribution to the measured events. Instead, we apply the method of moments that relies both on the orthogonality of angular functions and the estimation of integrals by Monte Carlo techniques. The big advantage of this method is that the joint distribution of *all* observables can be easily extracted, even for very few events. The method of moments is shown to be robust against mismodeling of the angular distribution. Our main result is an explicit algorithm that accounts for systematic uncertainties from detector-resolution and acceptance effects. Finally, we present the necessary process-dependent formulae needed for direct application of the method to several rare decays of interest.

I. INTRODUCTION

Our initial motivation for studying what we wish to call the *method of moments* is the determination of angular observables in the rare FCNC-mediated decay $\bar{B} \rightarrow \bar{K}^*(\rightarrow \bar{K}\pi)\ell^+\ell^-$. However, the method we describe in the following is general and applies to all decay or scattering processes that can be formulated in terms of an orthogonal basis of angular functions. We find a previous work [1] that advocates this method chiefly for the determination of angular observables in non-leptonic B decays but also mentions the applicability to semileptonic decays. Our aim is to improve upon this previous work by studying the uncertainties that are introduced by mismodeling of the angular distribution, and by working out a recipe to determine and unfold detector effects. The latter is crucial for the application of the method to real data. We show that the method of moments has several major advantages over the usual approach based on likelihood fits:

1. Likelihood fits have convergence problems for a small number of events, and can require reparametrizations and/or approximations for a successful fit to the signal PDF. As an example, see the LHCb analysis of the angular distribution in $\bar{B} \rightarrow \bar{K}^*\mu^+\mu^-$ decays [2].

The method of moments does not require any such reparametrizations or approximations.

2. Likelihood fits can be unstable in case the underlying physical model is only partially known. This can lead to overestimating the number of physical parameters, and consequently inhibits the convergence of the fits. As an example, this type of problem occurred in toy studies of the decay $B \rightarrow K^*(\rightarrow K\pi)\ell^+\ell^-$ as reported in [3]. It was subsequently solved when a missing symmetry relation between the angular observables was found and applied, thereby reducing the number of fit parameters.

In contrast, we will show that the method of moments does not require information on the correlations between model parameters as an input. Instead, it yields the correlations as an output, at the expense of somewhat larger uncertainties.

3. Mismodeling the underlying physics model can result in systematic bias in likelihood fits.

We will show that the method of moments is insensitive to a certain type of mismodeling; i.e. introducing a cutoff in a partial-wave expansion of the signal PDF.

4. Using the method of moments, the joint probability distribution of the angular observables rapidly converges towards a multivariate Gaussian distribution. This allows an easy transfer of correlation information from the experiments to interested theorists.

We continue with basic definitions that pertain to angular observables, and our results in the subsequent sections. Let $\vec{\vartheta}$ denote the set of all angles, and let \vec{v} denote the set of all other non-angular kinematic variables

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needed to fully specify the final state of the process under study. For example, $\vec{\nu}$ may include invariant masses or center-of-mass energies. We define an angular observable S_i as a coefficient in the probability density function (PDF), $P(\vec{\nu}, \vec{\vartheta})$, of the process by

$$P(\vec{\nu}, \vec{\vartheta}) \equiv \sum_i S_i(\vec{\nu}) \times f_i(\vec{\vartheta}). \quad (1)$$

Here, the dependence on the decay angles $\vec{\vartheta}$ has been explicitly factored out in terms of the angular functions $\{f_i(\vec{\vartheta})\}$. We assume there exists a dual basis of functions $\{\tilde{f}_i(\vec{\vartheta})\}$ such that the orthonormality relations

$$\int_{\Omega} d\vec{\vartheta} \tilde{f}_i(\vec{\vartheta}) f_j(\vec{\vartheta}) = \delta_{ij} \quad (2)$$

hold with Ω representing the full angular phase space relevant to the process. For particle decays, P is generally expressed in terms of the fully differential decay width,

$$P(\vec{\nu}, \vec{\vartheta}) \equiv \frac{1}{\Gamma} \frac{d^2\Gamma}{d\vec{\nu} d\vec{\vartheta}}, \quad (3)$$

where Γ is the total decay width. For a scattering process, one can similarly use

$$P(\vec{\nu}, \vec{\vartheta}) \equiv \frac{1}{\sigma} \frac{d^2\sigma}{d\vec{\nu} d\vec{\vartheta}}, \quad (4)$$

where the total cross section σ is used for the normalization. Since the determination of the total decay width or total cross section can be quite difficult, we emphasize that different normalizations for P can be used. For instance, the total decay width (or cross section) of the process of interest can be replaced by the corresponding quantity of a control-channel process. This change of normalization is equivalent to a linear rescaling of the angular observables $\{S_i\}$; thus ratios or similar suitable combinations of the angular observables are not affected by a change of normalization.

Our method is an extension of the classical method of moments with orthogonal functions [4, sec. 8.2]. The only difference is that conventionally the angular functions are assumed *self-dual*, $\tilde{f}_i = f_i$. However, it suffices that the system of angular functions $\{f_i(\vec{\vartheta})\}$ can be transformed into an orthonormal basis. We find it convenient to work in the basis of Legendre polynomials that are not self-dual. Our approach covers the self-dual case, provided that one replace $\tilde{f}_i \rightarrow f_i$ appropriately. Using the ansatz

$$\tilde{f}_i = \sum_j a_{ij} f_j, \quad (5)$$

the dual basis needs to be worked out case by case through solving the linear system of equations (2). For a selection of hadron decays with a b quark in the initial

state and two leptons in the final state, we list the dual bases in a series of appendices A through C. Note that a similar analysis was done in [1] for the decays $B \rightarrow J/\psi\phi$ and $B \rightarrow J/\psi K^*$.

In the remainder of this letter we discuss how to obtain an angular observable $S_i(\vec{\nu})$ in an experimental setup where each recorded event is (approximately) distributed according to P . We establish the statistical basics in section II. Section III is dedicated to the impact of systematic effects such as mismodeling the underlying physics or detector acceptance effects. Numerical studies for one uni-angular and one triple-angular distribution are provided in section IV.

II. SAMPLE-BASED DETERMINATION

The orthonormality relations eq. (2) imply that a single angular observable S_i can be projected out of the full PDF P as

$$S_i(\vec{\nu}) = \int_{\Omega} d\vec{\vartheta} P(\vec{\nu}, \vec{\vartheta}) \tilde{f}_i(\vec{\vartheta}). \quad (6)$$

where $\{\tilde{f}_i\}$ denotes a *dual basis* of angular functions, and Ω represents the entire angular phase space. In general, $\{\tilde{f}_i\}$ may differ from $\{f_i\}$. This is the case for our selection of applications in appendices A through C.

It is sensible to refer to the angular observable S_i as the f_i -moment of the PDF P . We emphasize that a relation of type eq. (6) holds for any combination of a density written as in eq. (1) and an orthonormal basis of angular functions $\{f_i\}$; *i.e.*, there is no unique basis of angular functions. For the proof we refer to ref. [1].

Integration over the non-angular variables yields

$$\langle S_i \rangle \equiv \int d\vec{\nu} S_i(\vec{\nu}) = \int d\vec{\nu} \left[\int_{\Omega} d\vec{\vartheta} P(\vec{\nu}, \vec{\vartheta}) \tilde{f}_i(\vec{\vartheta}) \right]. \quad (7)$$

The remainder of this section describes the method of moments, in which we replace the analytical integration by Monte Carlo (MC) estimates. The central tenet of MC integration is the fact that the expectation value $E_P[g]$ of some function $g(x)$ under the probability density $P(x)$,

$$E_P[g] \equiv \int dx P(x) g(x), \quad (8)$$

can be approximated by the consistent and unbiased estimator $\widehat{E_P[g]}$ [4, sec. 8.2]

$$E_P[g] \rightarrow \widehat{E_P[g]} \equiv \frac{1}{N} \sum_{n=1}^N g(x^{(n)}), \quad x^{(n)} \sim P \quad (9)$$

due to the strong law of large numbers for $N \rightarrow \infty$, assuming that the variates $x^{(n)}$, $n = 1, \dots, N$, are distributed as P . Throughout this letter we denote all

MC estimators with a wide hat.

Application of eq. (9) then yields

$$\langle S_i \rangle \rightarrow \widehat{\langle S_i \rangle} = \frac{1}{N} \sum_{n=1}^N \tilde{f}_i(x^{(n)}). \quad (10)$$

It is often of interest to obtain observables integrated over certain bins of $\vec{\nu}$. We define

$$\langle S_i \rangle_{\vec{a}, \vec{b}} \equiv \int_{\vec{a}}^{\vec{b}} d\vec{\nu} S_i(\vec{\nu}) \quad (11)$$

$$\begin{aligned} &= \int_{\vec{a}}^{\vec{b}} d\vec{\nu} \left[\int_{\Omega} d\vec{\vartheta} P(\vec{\nu}, \vec{\vartheta}) \tilde{f}_i(\vec{\vartheta}) \right] \\ &= \int d\vec{\nu} \left[\int_{\Omega} d\vec{\vartheta} P(\vec{\nu}, \vec{\vartheta}) \tilde{f}_i(\vec{\vartheta}) \mathbf{1}(\vec{a} \leq \vec{\nu} \leq \vec{b}) \right], \end{aligned} \quad (12)$$

$$(13)$$

where the argument of the indicator function $\mathbf{1}(\vec{a} \leq \vec{\nu} \leq \vec{b})$ is to be interpreted componentwise. Application of eq. (9) immediately yields

$$\widehat{\langle S_i \rangle}_{\vec{a}, \vec{b}} = \frac{1}{N} \sum_{n=1}^N \tilde{f}_i(x^{(n)}) \mathbf{1}(\vec{a} \leq \vec{\nu} \leq \vec{b}). \quad (14)$$

For notational simplicity, let us forget about the $\vec{\nu}$ integration and consider only S_i . In the limit $N \rightarrow \infty$, the central limit theorem (CLT) implies that the random vector

$$\widehat{\vec{S}} \equiv (\widehat{S}_0, \dots, \widehat{S}_i, \dots) \quad (15)$$

follows a multivariate Gaussian distribution $\mathcal{N}(\vec{S}, \Sigma)$ centered on the true value \vec{S} with the covariance Σ_{ij} estimated as

$$\begin{aligned} \Sigma_{ij} &\equiv \text{Cov}[S_i, S_j] \\ &\rightarrow \widehat{\Sigma}_{ij} \equiv \widehat{\text{Cov}}[S_i, S_j] \\ &= \frac{1}{N-1} \sum_{n=1}^N \left[\tilde{f}_i(x^{(n)}) - \widehat{S}_i \right] \left[\tilde{f}_j(x^{(n)}) - \widehat{S}_j \right]. \end{aligned} \quad (16)$$

In our physics applications, the parameter space is compact and each \tilde{f}_i is bounded. Hence the requisites for the most basic version of the CLT to hold — finite mean and covariance of \tilde{f}_i — are automatically satisfied. In our numerical analysis the sample covariance rapidly converges towards the true covariance matrix; see also section IV.

Compared to the usual maximum-likelihood approach, we find for the method of moments:

1. The angular observable S_i can be determined independently of any other observable S_j . It is therefore much more robust to physics assumptions needed to define the full likelihood. In particular, this means

one does not have to be specific regarding the form of new-physics contributions; in fact, one does not even need to be able to explicitly formulate the likelihood at all.

2. It is superior for a small number of samples N . Likelihood fits tend to be numerically unstable if lots of parameters need to be estimated from sparse data. This is more severe if the mode of the likelihood is near the boundary of the physically allowed region [5]. For some of these decays of interest, there are only $\mathcal{O}(100)$ events recorded per bin.
3. The estimate is unbiased for any N . In contrast, the maximum-likelihood estimate has a bias of order $1/N$ [6]. In practice, one should keep in mind the bias-variance trade-off: it is a well known phenomenon that removing the bias usually leads to an increase in variance of the sampling distribution of the estimator and vice versa [4, sec. 7.3]. From a Bayesian decision-theory point of view, both contribute similarly to the expected loss associated with deciding on just one value of the unknown parameter. One should therefore not prefer the method of moments over likelihood fits just because the former reduces the bias [7, sections 13.8, 17.2]. In fact, for the results discussed below in section IV, the likelihood fits — if they converge — exhibit a negligible bias and produce uncertainties 10%–30% smaller than those from the method of moments.
4. The approximate multivariate Gaussian distribution of $\widehat{\vec{S}}$ allows easier and more precise transfer of the information in the data to interested theorists for more accurate fits of standard-model and new-physics parameters [8–10], or for more precise predictions of optimized observables; see e.g., [11–17] for definitions of such optimized observables in $B \rightarrow K^* \ell^+ \ell^-$ decays, [18] for application to the decay $B \rightarrow \pi \pi \ell^+ \ell^-$, and [19] for observables in $\Lambda_b \rightarrow \Lambda(\rightarrow N\pi) \ell^+ \ell^-$. While the likelihood also approaches a multivariate Gaussian as $N \rightarrow \infty$, the two methods differ in their utility as input for theorists if $\widehat{\vec{S}}$ is not well inside the physical region. For example, suppose there are two angular observables that are constrained to a triangular region by phase-space or unitarity arguments as

$$|S_1| + S_2 \leq 1, \quad S_1 \in [-1, 1], \quad S_2 \in [0, 1]. \quad (17)$$

It may (and often does) happen in practice that $\widehat{\vec{S}}$ is close or even outside the allowed region such that a significant part of the probability mass covers unphysical values. In a Bayesian fit, one would take $\mathcal{N}(\widehat{\vec{S}} | \vec{S}, \widehat{\Sigma})$ as the sampling distribution of the “data”, and simply set a uniform prior on the triangle in the \vec{S} plane defined by eq. (17) to have a well defined problem. This could be trivially

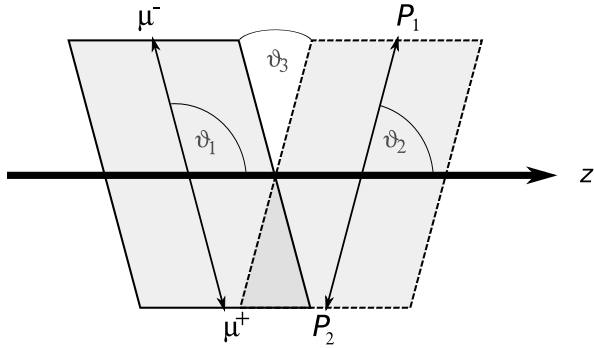


FIG. 1. Decay topology for decays $B \rightarrow P_1 P_2 \ell_1 \bar{\ell}_2$.

combined with other independent information in a global fit. Someone with a different physics model might have to consider a different physical region, and could incorporate it just as easily.

For a likelihood fit, the constraint needs to be part of the analysis performed by the experimental collaboration, and the resulting likelihood as a function of \vec{S} may be distinctly not Gaussian. Communicating such a result has proved to be challenging due to technical reasons (such as data formats, size etc.) This leads to the undesirable situation that only the mode and standard errors are reported, and theorists often include the results as independent measurements with a Gaussian distribution and disregard the boundary problem as well as correlations altogether.

III. SOURCES OF SYSTEMATIC UNCERTAINTIES

In section II, we assume that the PDF P describes the underlying physics accurately, and that the experiment observes each event with perfect accuracy. In order to estimate systematic uncertainties, we lift these assumptions.

A. Mismodeling due to Contributions by Higher Partial Waves

In several interesting processes we might only have an approximate result for P . In this section, we focus on one particular class of mismodeling of the signal PDF: the angular-momentum cutoff in partial-wave expansions. This mismodeling potentially affects a large number of decays and scattering processes. For the sake of clarity we take the interesting class of four-body

decays $B \rightarrow P_1 P_2 \ell_1 \ell_2$ as an example¹.

Within existing analyses, the PDFs of these decays are usually expressed in terms of one or a few partial waves of the dimeson system. However, the angular momentum of the dimeson system is unbounded from above, and gives rise to an infinite set of angular observables.

For the selected class of decays, we can describe that problem as follows: The PDF P has a fixed dependence on the dilepton helicity angle ϑ_1 and the azimuthal angle ϑ_3 . (See also appendix C for details on the angular distribution.) However, at the level of decay amplitudes the dimeson system can have an arbitrarily large total angular momentum j ; only its third component is restricted to $j_z = -1, 0, +1$. It is then convenient to compute the angular distribution explicitly in terms of ϑ_1 and ϑ_3 , but leave the angular observables dependent on the remaining helicity angle ϑ_2 of the dimeson:

$$P(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3) \equiv \sum_k S_k(\vec{\nu}, \cos \vartheta_2) f_k(\cos \vartheta_1, \vartheta_3). \quad (18)$$

We advocate here that is a sensible procedure to perform an expansion in terms of Legendre polynomials $p_l^{(|m|)}$ with respect to the remaining angle ϑ_2 . Here, the angular-momentum indices l and m follow from the usual rules for addition of the angular momenta j and \tilde{j} of the partial-wave expansion of the underlying amplitude and its complex conjugate: $j - \tilde{j} \leq l \leq j + \tilde{j}$, and $m = j_z + \tilde{j}_z$.

For the decay at hand, we consider the partial-wave expansion for the angular observables (see [22] and appendix D)

$$S_k(\vec{\nu}) \equiv \frac{I_k(\vec{\nu})}{4\pi\Gamma}, \quad \text{with} \quad \Gamma = I_1(\vec{\nu}) - \frac{I_2(\vec{\nu})}{3}, \quad (19)$$

which reads

$$S_k(\vec{\nu}, \cos \vartheta_2) \equiv \sum_{l=0}^{\infty} \frac{1}{n_{l,|m|}} S_{k,l}(\vec{\nu}) p_l^{(|m|)}(\cos \vartheta_2). \quad (20)$$

The normalization factor $n_{l,|m|}$ is defined in eq. (D3). Within our example we have (cf. also appendix C and [22])

$$|m| = \begin{cases} 0, & k = 1, 2, 6 \\ 1, & k = 4, 5, 7, 8 \\ 2, & k = 3, 9 \end{cases}. \quad (21)$$

¹ This includes the rare $b \rightarrow s$ mediated B decay $B \rightarrow K\pi\ell^+\ell^-$, and the V_{ub} suppressed decay $B \rightarrow \pi\pi\ell^+\bar{\nu}_\ell$. For both examples the PDF P is known in the small-width approximation and when assuming a pure P -wave resonant final state. An extension to $S - P$ interference has been studied for $B \rightarrow K\pi\ell^+\ell^-$ [14, 20], and for $\bar{B} \rightarrow \pi\pi\ell^-\bar{\nu}_\ell$ [18]. For a first study of S , P and D interference, see [21]

The angular observables $S_{k,l}$ – as defined in eq. (20) – have the merit of a well defined total angular momentum, and thus are physically distinguishable. As a consequence of the orthogonality of the Legendre polynomials, any mismodeling (or rather, lack of modelling) of higher partial-wave observables *does not affect* the method of moments as discussed in the previous section. That is to say, adding further (orthogonal) terms to the PDF only appends observables to \vec{S} , but does not change the leading elements. The same applies to the covariance.

Unfortunately, this benefit on the experimental side is accompanied with a theoretical drawback. Each observable $S_{k,j}(\vec{v})$ consists of an infinite sum of bilinears of partial-wave amplitudes. It remains for theoretical analyses to estimate or calculate the impact of partial waves beyond the S and P wave contributions. (For $B \rightarrow K\pi^+\ell^-$ a first study has been carried out where contributions up to the D wave are investigated [21]).

We wish to emphasize that detector acceptance effects systematically affect the expansion for any basis of angular functions, including the one suggested in this section. Nevertheless, the expansion in terms of Legendre polynomials as suggested above provides means to cope with these effects, as we discuss in the following subsection.

B. Recipe for Including Detector Effects

Ascertaining a detector's performance to detect signal events with accurate determination of the event's angles is generally a difficult task. In the ideal case, one would have an explicit probabilistic model of the detector acceptance and could thus write down the full forward model from which the measured events arise. In practice, that is not feasible, and one is forced to simplify the model. The standard approach is to generate the *true* particle events $\{x_t^{(n)}\} = \{(\vec{v}_t^{(n)}, \vec{\vartheta}_t^{(n)})\}$, $n = 1, \dots, N_t$, from a PDF assumed to describe the bare physical process, and to propagate those particles through a detailed simulation of the detector. The observable traces that the particles leave in the detector are fed into reconstruction algorithms resulting in the *detector* events $\{x_d^{(n)}\} = \{(\vec{v}_d^{(n)}, \vec{\vartheta}_d^{(n)})\}$, $n = 1, \dots, N_d$ with $N_d \leq N_t$. In general, the distribution of the detected events is

$$P_d(x_d) = \frac{1}{R} \int dx_t P_t(x_t) E(x_d|x_t). \quad (22)$$

Here P_t is the probability distribution of the true events, the normalization constant R is given by

$$R \equiv \iint dx_t dx_d P_t(x_t) E(x_d|x_t). \quad (23)$$

The kernel $E(x_d|x_t)$ is usually decomposed as

$$E(x_d|x_t) = \varepsilon(x_t) P(x_d|x_t), \quad (24)$$

where the PDF $P(x_d|x_t)$ models the resolution effects and the unnormalized density $\varepsilon(x_t)$ is the *detector acceptance* function. Perfect resolution corresponds to

$$P(x_d|x_t) = \delta(x_d - x_t). \quad (25)$$

In what follows, we propose a systematic method to unfold all effects of $E(x_d|x_t)$ through MC simulations and the method of moments, using that $E(x_d|x_t)$ can be expanded — at least formally — in Legendre polynomials. For illustration, we proceed with the explicit example of a uniangular² PDF with $x = \cos \vartheta$. Let us define the PDF in terms of the Legendre polynomials (i.e., $f_k(x) \equiv p_k(x)$) and angular observables \vec{S} as

$$P_t(x_t) \equiv P_t(x_t|\vec{S}) = \sum_k S_k f_k(x_t), \quad (26)$$

where $k = 0, 1, \dots$ denotes an angular-momentum-like index associated with the observables. Normalization of P_t is equivalent to choosing $S_0 = 1/2$. Requiring $P_t(x_t) \geq 0 \forall x_t$ implies $|S_k| \leq 1/2$ for $k > 0$. More stringent relations between the S_k might hold, but are of no concern here. For later use, we define

$$S_k^{(m)} \equiv \begin{cases} 1/2\delta_{k,0}, & m = 0 \\ 1/2(\delta_{k,0} + \delta_{k,m}), & m > 0, \end{cases} \quad (27)$$

and note that

$$P^{(m)}(x_t) \equiv P(x_t|\vec{S}^{(m)}) \quad (28)$$

is a valid PDF. The dual basis of angular functions follows then from the normalization and orthogonality of the Legendre polynomials, and one therefore has

$$\tilde{f}_k(x) = \frac{2k+1}{2} f_k(x), \quad (29)$$

$$\int_{-1}^{+1} dx \tilde{f}_k(x) f_l(x) = \delta_{k,l}. \quad (30)$$

We now define the *simulated raw* moments $\vec{Q}^{(m)}$ as

$$Q_i^{(m)} \equiv \iint dx_t dx_d \tilde{f}_i(x_d) P^{(m)}(x_t) E(x_d|x_t), \quad (31)$$

which are instrumental to our recipe. Monte Carlo estimators of these moments can be constructed from specifically crafted detector events $x_d^{(n,m)}$, $n = 1, \dots, N_d^{(m)}$, where

$$x_d^{(n,m)} \sim P_E^{(m)}(x_d) \equiv \frac{1}{R^{(m)}} \int dx_t P^{(m)}(x_t) E(x_d|x_t). \quad (32)$$

² The generalization of this section to multiangular PDFs is straightforward. It can be achieved by promoting x to a vector, promoting the Legendre polynomials to products of independent polynomials or spherical harmonics, and promoting the indices i, j, k, m to multi-indices.

In words, for each m it is required to generate events from a toy physical distribution $P^{(m)}$, for which $S_0 = S_m = 1/2$ and all other observables are set to zero. Next, propagate these events through a detector simulation. The normalization $R^{(m)}$ is chosen such that $\int P_E^{(m)}(x_d) dx_d = 1$. We emphasize that $R^{(m)}$ can be estimated as $\hat{R}^{(m)} = N_d^{(m)}/N_t$, where N_t corresponds to the number of simulated true events. The estimators then read

$$\hat{Q}_i^{(m)} \equiv \hat{R}^{(m)} \frac{1}{N_d} \sum_n \tilde{f}_i(x_d^{(n,m)}) \quad (33)$$

Linearity of the integral over x and convergence of the expansion of $P_E^{(m)}$ in terms of Legendre polynomials ensures that

$$\vec{Q}^{(m)} = M \vec{S}^{(m)}. \quad (34)$$

We call the matrix M^{-1} the *unfolding matrix*, which is specific to the decay at hand. Given our definition of $S_k^{(m)}$ in eq. (27) it is easy to see that

$$M_{ij} = \begin{cases} 2Q_i^{(0)} & j = 0, \\ 2(Q_i^{(j)} - Q_i^{(0)}) & j \neq 0, \end{cases} \quad (35)$$

and its MC estimator \hat{M} can be obtained through the replacements $Q_i^{(m)} \rightarrow \hat{Q}_i^{(m)}$.

In order to finally extract the angular observables from data, we use the *measured raw moments*. Their MC estimator $\hat{\vec{Q}}$ — based on the *detected events* $x^{(n)}$, $n = 1, \dots, N$ — reads

$$\hat{Q}_i \equiv R \frac{1}{N} \sum_n \tilde{f}_i(x^{(n)}). \quad (36)$$

We then obtain MC estimators of the angular observables via

$$\hat{\vec{S}} \equiv [\hat{M}^{-1}] \hat{\vec{Q}}. \quad (37)$$

Apparently we now face a circular dependence. On the one hand, the estimators $\hat{\vec{Q}}$ and thus also $\hat{\vec{S}}$ are proportional to R , the ratio of detected events over occurring events. On the other hand, R depends by construction (see eq. (23)) on $P_t(x_t)$, and thus on the true value of the angular observables \vec{S} . This dependence is broken by the fact that the MC estimators $\hat{\vec{S}}$ need to fulfill the self-consistency condition

$$\hat{S}_0 = \frac{1}{2}, \quad \text{for a uniaxial distribution.} \quad (38)$$

(For the process-dependent conditions in the multiangular case see eq. (B9) and eq. (C6).) This self-consistency

condition is tightly related to the determination of the branching ratio of the underlying decay, and we therefore suggest to carry out a combined analysis for the determination of the branching ratio and the extraction of the angular observables. Moreover, in the applications to B decays only ratios and similar R -independent combinations of the angular observables are of interest.

We note that $\hat{\vec{S}}$ as determined from eq. (37) does not fully correspond to \vec{S} for arbitrary detector acceptance ε . Assuming an expansion of ε in terms of Legendre polynomials up to a given order L , we have to calculate the raw moments up to $\dim \hat{\vec{Q}} = \dim \hat{\vec{S}} = \dim S + L$. The MC estimators of the corrected angular observables then take the following structure:

$$\hat{\vec{S}} = (\underbrace{\hat{S}_0, \dots, \hat{S}_{\dim S-1}}_{\text{physical}}, \underbrace{\hat{S}_{\dim S}, \dots, \hat{S}_{\dim Q-1}}_{\text{“superfluous”}}). \quad (39)$$

The method is consistent as long as the MC estimators for the “superfluous” observables are compatible with zero.³ The value L depends on the setup of the particle detector under consideration, and remains to be determined just as in studies that carry out a likelihood fit.

The accuracy of the unfolding process as outlined above critically depends on both the accuracy of the detector simulation, as well as the uncertainties induced by the MC estimates. For an experimental analysis, one would now turn to the determination of the distribution of \vec{S} as a function of the detector setup. This would involve the determination of both M and \vec{Q} for a number of detector configurations, and subsequent profiling or marginalization. While such considerations of any detector simulation are beyond the scope of this work, we can, however, comment on the MC-induced uncertainties. As usual, one needs to find a balance between compute time and accuracy. For a uniaxial distribution and $\mathcal{O}(10^6)$ MC samples, we find that the error on the mean of each matrix element is $\mathcal{O}(10^{-4})$. This suggests that the so-induced systematic error can be driven below any statistical uncertainty.

An alternative method to unfold detector effects is weighting the data on an event-by-event basis, with each weight corresponding to the inverse of the detection efficiency.

³ This holds only for the physical model of uniaxial decay distributions. If the physical model involves a partial-wave expansion with cutoff, these superfluous observables correspond to higher partial waves that have been suppressed in the physical model; see appendix C for such a case.

Let us conclude this section by commenting that parts of the unfolding matrix are universal in a sense: They can be reused in analyses with a similar underlying decay. Therefore, computing resources spent on improving the accuracy of \widehat{M} are not wasted.

IV. TOY STUDIES

We now study the performance of the proposed method. In order to do so, we simulate individual events for two separate physical processes: one uni-angular, and one tri-angular decay distribution. We repeat the analysis for varying sample sizes, ranging from 50 to 500 events. Our toy analyses are based on SM predictions for angular observables in the decays $B \rightarrow K\ell^+\ell^-$ and $B \rightarrow K^*(\rightarrow K\pi)\ell^+\ell^-$. In order to faithfully investigate the performance of the method of moments, we repeat our numerical studies for several bins in the kinematic range $1\text{ GeV}^2 \leq q^2 \leq 6\text{ GeV}^2$, as well as $15\text{ GeV}^2 \leq q^2 \leq q_{\text{max}}^2$. Here, the bin width is chosen either as 1 GeV^2 or 0.5 GeV^2 . This setup is meant to ensure that a wide spectrum of possible values for the angular observables is investigated.

Our findings can be summarized as follows:

- In all studied cases we observed not a single bias in the distribution of the pull of any observables S_i ,

$$\text{pull}_i \equiv \frac{\widehat{S}_i - S_i}{\widehat{\sigma}_i}. \quad (40)$$

Here S_i refers to the true (input) value for the angular observables, \widehat{S}_i refers to the mean of the pseudo measurement via the MC estimate, and $\widehat{\sigma}_i \equiv \widehat{\Sigma}_{ii}^{1/2}$ refers to an estimator of the standard deviation of the pseudo measurement. All pull distributions obtained in our studies can be successfully fitted to a Gaussian distribution. Out of the large number of studied distributions, we only show the pull distributions for the observables $S_5 \simeq 27\%$ and $S_7 \simeq 2\%$ obtained from SM-like $B \rightarrow K^*\ell^+\ell^-$ decays as representative examples. We generated $2 \cdot 10^5$ toy studies with 200 events per study in figure 2.

- We study the MC estimate for the absolute uncertainty $\widehat{\sigma}_i(N)$ with respect to the angular observable S_i as a function of the number of simulated events N . As expected for a multivariate Gaussian distribution, we find that the absolute uncertainty is well fitted by

$$\widehat{\sigma}_i(N) = \frac{\sigma_i}{\sqrt{N}} \quad (41)$$

with $\sigma_i(1) = \mathcal{O}(1)$, regardless of the absolute size of S_k . The latter can best be shown for the example of uncertainties of two observables. Taking again S_5

($\simeq 27\%$) and S_7 ($\simeq 2\%$) for SM-like $B \rightarrow K^*\ell^+\ell^-$ decays, we show the absolute uncertainty in figure 3. We find that the method of moments yields uncertainties on \vec{S} that are roughly 10% – 30% larger than those obtained from maximum-likelihood fits and for the same number of events. However, we wish to note that said fits only produce a limited subset of the angular observables, and the statistical error of the fit is expected to increase with the number of fit parameters until their errors saturate the statistical errors of the method-of-moments estimators [23, sec. 8].

- We also compare the results as obtained by the method of moments with results obtained by a conventional likelihood fit. In particular, we study the correlation between the method-of-moment estimators and the maximum-likelihood-fit estimators. We run 10^3 toy analyses, with 200 simulated events per analysis. We show the joint distribution of the two estimators in figure 4. The two estimators are highly correlated. The distribution of the difference of the estimators exhibits now

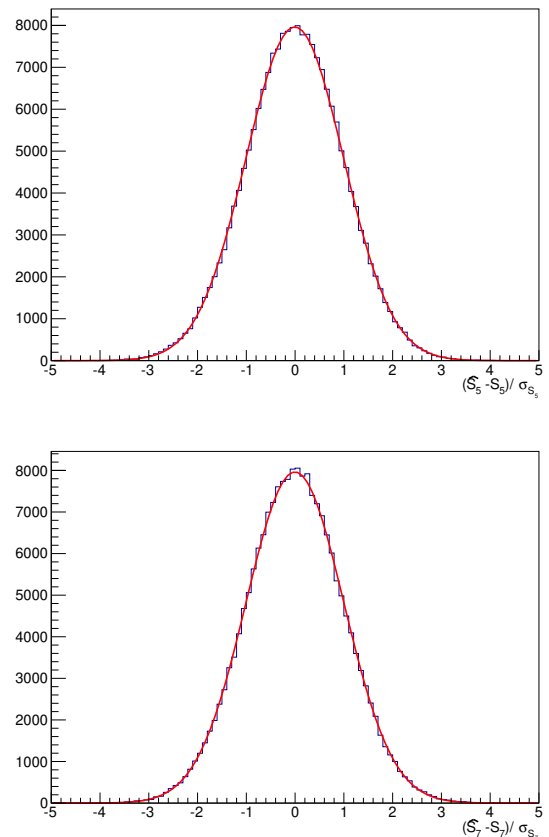


FIG. 2. Pull distribution for the angular observables S_5 (upper) and S_7 (lower), extracted from $2 \cdot 10^5$ studies of 200 simulated events each for the decay $B \rightarrow K^*\ell^+\ell^-$. The red curve represents a fit to a Gaussian distribution.

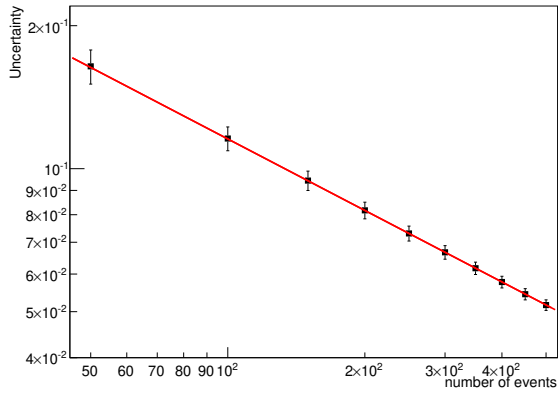


FIG. 3. Uncertainty $\hat{\sigma}_5$ of the angular observable S_5 extracted from $2 \cdot 10^5$ studies of simulated events for the decay $B \rightarrow K^* \ell^+ \ell^-$. We show the uncertainty as a function of the number of simulated events N . The red curve represents a fit to the function given in eq. (41). The error bars correspond to the 68% spread of measured uncertainties in the toys. The plot for $\hat{\sigma}_7$ is visually indistinguishable from the one shown here.

bias, which is due to the large number of simulated events. Still, we find that statistical uncertainty on the difference of the two estimators is sizeable and can easily become half as large as the statistical uncertainty of either estimator.

We emphasize that the above results have been obtained for a flat acceptance function. We also study the behavior of the unfolded angular observables. For simplicity we limit our study to the decay $B \rightarrow K \ell^+ \ell^-$, with its three angular observables S_0 to S_2 . We express the acceptance function in terms of Legendre polynomials $p_k(x)$,

$$\varepsilon(\cos \vartheta) = \frac{7}{15} p_0(\cos \vartheta) - \frac{4}{15} p_2(\cos \vartheta). \quad (42)$$

This acceptance function approximates the one used in a recent study of the angular observables in $B \rightarrow K \ell^+ \ell^-$ decays [24]. Focusing on effects of the unfolding process itself, we use the analytical expression for the unfolding matrix, which we compute from the raw moments as defined in eq. (31). Simulating 4000 toy analyses with up to 300 simulated events each, we find that the previous bullet points still hold; i.e., we do not find any bias, and the distribution is well described by a multivariate Gaussian distribution. The latter only holds as long as the number of events per experiment exceeds ~ 30 .

All of our toy studies, as summarized above, show consistently that the joint distribution of the angular observables converges rapidly towards a multivariate Gaussian distribution. We therefore propose to publish the results in the form of the physical components of $\hat{\mathcal{S}}$ and $\hat{\Sigma}$.

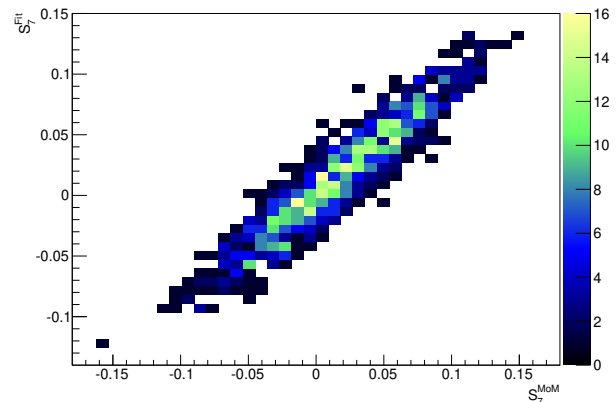
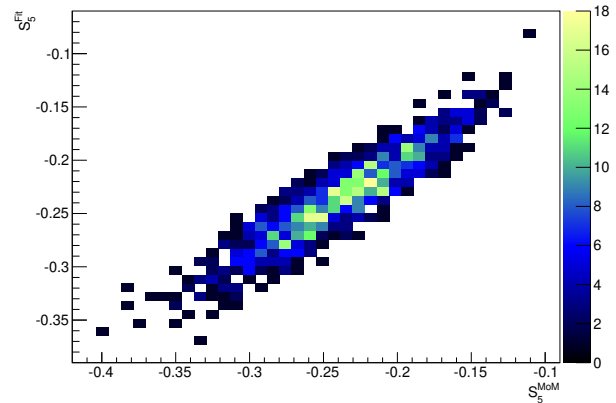


FIG. 4. The joint distribution of the two estimators \hat{S}_i^{MoM} and \hat{S}_i^{Fit} that arise from the method of moments and a maximum-likelihood fit, respectively. We show the estimators for both of our benchmark observables S_5 (upper) and S_7 (lower).

V. SUMMARY

We have carried out a combined analytical and numerical study of the method of moments; a method for the extraction of angular observables from the angular distribution of a general multi-body process. We have studied the performance of the method of moments using pseudo data derived from the SM predictions for one uniangular decay ($B \rightarrow K \ell^+ \ell^-$) and one triangular decay ($B \rightarrow K^* \ell^+ \ell^-$). From this, we find rapid convergence of the joint likelihood of the angular observables towards a multivariate Gaussian. We draw the conclusion that this method exhibits several benefits in the determination of angular observables when compared with a maximum-likelihood fit.

First, we find no bias in the determinations of the angular observables even for a small number of events. However, due to fewer model assumptions, the uncertainty on the mean values increases by roughly 10%–30% compared to likelihood fits. Second, in the absence of detector effects, the method

of moments does not rely on model assumptions for the partial-wave composition of the PDF. This is explicitly shown for the case of higher partial waves in multibody final states.

Third, we develop a systematic method for the determination of detector effects that lead to dilution and mixing of the angular observables. We present an algorithm to calculate the necessary unfolding matrix, which is computationally feasible only when using the method of moments. The algorithm also accounts for higher partial waves.

Fourth, the joint distribution of the angular observables resulting from the method of moments is well approximated by a multivariate Gaussian distribution even for small number of events $N \sim 30$ both for the ideal uniform acceptance and a realistic example. This facilitates the precise transfer of correlation information to subsequent theoretical analyses.

Last but not least, the resulting distribution arises without the need for additional model constraints. Thus more observables can be inferred from the same data than in a likelihood fit. In addition, the results from the method of moments can be more easily averaged or combined; e.g., in global fits.

In conclusion, we argue that the method of moments is a competitive alternative to maximum-likelihood fits if angular distributions are involved. We wish to raise the interesting prospect of extending this method to applications that feature PDFs composed from non-angular orthogonal bases.

ACKNOWLEDGMENTS

We thank Ulrik Egede for insightful discussions and helpful comments on the manuscript. We are grateful to Robert Fleischer, Gudrun Hiller, Martin Jung and Konstantinos Petridis for helpful discussions, as well as Claus Grupen for helpful advice in searching the literature. N.S. acknowledges the support of the Swiss National Science Foundation, PP00P2-144674. The work of D.v.D has been supported by the Bundesministerium für Bildung und Forschung (BMBF).

Appendix A: Application to $\bar{B} \rightarrow \bar{K} \ell^+ \ell^-$

The PDF for the decay $\bar{B} \rightarrow \bar{K} \ell^+ \ell^-$ has been calculated for the most complete basis of dimension-six

$b \rightarrow s \ell^+ \ell^-$ operators. It reads [15, 25]

$$\begin{aligned} P(q^2, \cos \vartheta_1) &= \frac{1}{d\Gamma/dq^2} \frac{d^2\Gamma}{dq^2 d\cos \vartheta_1} \\ &= \frac{a(q^2)}{d\Gamma/dq^2} + \frac{b(q^2)}{d\Gamma/dq^2} \cos \vartheta_1 \\ &\quad + \frac{c(q^2)}{d\Gamma/dq^2} \cos^2 \vartheta_1 \\ &\equiv \sum_i S_i p_i(\cos \vartheta_1), \end{aligned} \quad (\text{A1})$$

with the conventional observables $a(q^2)$ through $c(q^2)$, and $d\Gamma/dq^2 = 2a + 2/3c$. We conveniently use the Legendre polynomials $p_i(x)$, $i = 0, 1, 2$,

$$p_0(x) = 1, \quad p_1(x) = x, \quad p_2(x) = \frac{1}{2}(3x^2 - 1), \quad (\text{A2})$$

as our basis of angular functions. Our basis of angular observables then translates to the conventional basis as

$$S_0 = \frac{1}{2}, \quad S_1 = \frac{b}{\Gamma}, \quad S_2 = \frac{2c}{3\Gamma}. \quad (\text{A3})$$

In this case, the dual basis is simply given by $\tilde{p}_i(x) = (2i+1)/2p_i(x)$ such that

$$\int_0^\pi d\vartheta_1 \tilde{p}_i(\cos \vartheta_1) P(q^2, \cos \vartheta_1) \sin \vartheta_1 = S_i(q^2). \quad (\text{A4})$$

Appendix B: Application to $\Lambda_b \rightarrow \Lambda(\rightarrow N\pi) \ell^+ \ell^-$

The PDF for the decay — in the presence of Standard-Model operators and their chirality-flipped counter parts — reads [19]

$$\begin{aligned} P(q^2, \cos \vartheta_1, \cos \vartheta_2, \vartheta_3) &= \frac{(d\Gamma/dq^2)^{-1} d^4\Gamma}{dq^2 d\cos \vartheta_1 d\cos \vartheta_2 d\vartheta_3} \\ &= \sum_i S_i f_i(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3), \end{aligned} \quad (\text{B1})$$

where q^2 denotes the dilepton mass squared, $\vartheta_1 \equiv \vartheta_\ell$ and $\vartheta_2 \equiv \vartheta_\Lambda$ denote the helicity angles in the dilepton and $N\pi$ systems, respectively, and $\vartheta_3 = \phi$ denotes the azimuthal angle. The index i should be interpreted as a multi-index, $i \equiv (l_1, l_2, m)$, where $0 \leq l_1 \leq 2$ and $0 \leq l_2 \leq 1$ denote the total angular momentum in the dilepton and the $N\pi$ system, respectively, and $-1 \leq m \leq 1$ is the third component of either of the angular momenta.

Our choice of an orthonormal basis reads

$$\begin{aligned} f_{l_1, l_2, m}(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3) \\ = \sqrt{\frac{(l_1 - |m|)! (l_2 - |m|)!}{(l_1 + |m|)! (l_2 + |m|)!}} \end{aligned}$$

$$\begin{aligned}
& \times p_{l_1}^{|m|}(\cos \vartheta_1) p_{l_2}^{|m|}(\cos \vartheta_2) \\
& \times \begin{cases} \cos(|m|\vartheta_3) & m > 0 \\ \sin(|m|\vartheta_3) & m < 0 \\ 1 & m = 0 \end{cases}, \quad (\text{B2})
\end{aligned}$$

$$\begin{aligned}
& = \frac{(2l_1+1)(2l_2+1)}{8\pi} \sqrt{\frac{(l_1-m)!(l_2-m)!}{(l_1+m)!(l_2+m)!}} \\
& \times p_{l_1}^m(\cos \vartheta_1) p_{l_2}^m(\cos \vartheta_2) \\
& \times \begin{cases} 2 \cos(|m|\vartheta_3) & m > 0 \\ 2 \sin(|m|\vartheta_3) & m < 0 \\ 1 & m = 0 \end{cases}.
\end{aligned}$$

and its dual is

$$\tilde{f}_{l_1, l_2, m}(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3)$$

The correspondence between our choice of angular observables in the angular momentum basis, and the angular observables as defined in reference [19] reads

$$8\pi S_{0,0,0} = 1, \quad 8\pi S_{0,1,0} = \frac{K_{2cc} + 2K_{2ss}}{d\Gamma/dq^2}, \quad (\text{B4})$$

and

$$\begin{aligned}
8\pi S_{1,1,-1} &= \frac{6K_{4s}}{d\Gamma/dq^2}, \\
8\pi S_{1,0,0} &= \frac{3K_{1c}}{d\Gamma/dq^2}, \quad 8\pi S_{1,1,0} = \frac{3K_{2c}}{d\Gamma/dq^2}, \\
8\pi S_{1,1,+1} &= \frac{6K_{3s}}{d\Gamma/dq^2},
\end{aligned} \quad (\text{B5})$$

and

$$\begin{aligned}
8\pi S_{2,1,-1} &= \frac{2\sqrt{3}K_{4sc}}{d\Gamma/dq^2}, \\
8\pi S_{2,0,0} &= \frac{2(K_{1cc} - K_{1ss})}{d\Gamma/dq^2}, \quad 8\pi S_{2,1,0} = \frac{2(K_{2cc} - K_{2ss})}{d\Gamma/dq^2}, \\
8\pi S_{2,1,+1} &= \frac{2\sqrt{3}K_{3sc}}{d\Gamma/dq^2},
\end{aligned} \quad (\text{B6})$$

where the decay width is

$$\frac{d\Gamma}{dq^2} = 2K_{1ss} + K_{1cc}. \quad (\text{B7})$$

The dual basis is chosen such that

$$\int_{-1}^{+1} d\cos \vartheta_1 \int_{-1}^{+1} d\cos \vartheta_2 \int_0^{2\pi} d\vartheta_3 P(q^2, \cos \vartheta_1, \cos \vartheta_2, \vartheta_3) \tilde{f}_i(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3) = S_i(q^2). \quad (\text{B8})$$

For the purpose of unfolding acceptance effects as laid down in section III B, it is instrumental to know that $f_{0,0,0} \equiv 1$, and that $\max_{\cos \vartheta_1, \cos \vartheta_2, \phi} |f_{l_1, l_2, m}| < 1$.

The recipe's generating PDFs are therefore $P(x|\{S_i^{(j)}\})$, with

$$S_i^{(j)} = \frac{1}{8\pi} \begin{cases} \delta_{i,(0,0,0)} & j = (0,0,0) \\ \delta_{i,(0,0,0)} + \delta_{i,j} & j \neq (0,0,0) \end{cases}, \quad (\text{B9})$$

and where j is now also a multi-index representing $j \equiv (\tilde{l}_1, \tilde{l}_2, \tilde{m})$.

Appendix C: Application to $\bar{B} \rightarrow \bar{K} \pi \ell^+ \ell^-$

The PDF for the decay $\bar{B} \rightarrow \bar{K} \pi \ell^+ \ell^-$ — up to and including P-wave contributions — has been calculated for the most general basis of dimension-six $b \rightarrow s$ operators.

It reads, expressed in terms of the angular observables $\{J_i\}$ [15, 20]

$$P(q^2, \cos \vartheta_1, \cos \vartheta_2, \vartheta_3) = \frac{(d\Gamma/dq^2)^{-1} d^4\Gamma}{dq^2 d\cos\vartheta_1 d\cos\vartheta_2 d\vartheta_3} = \sum_i S_i(q^2) f_i(\cos \vartheta_1, \cos \vartheta_2, \vartheta_3), \quad (C1)$$

where $\vartheta_1 \equiv \vartheta_\ell$ is the dilepton helicity angle; $\vartheta_2 \equiv \vartheta_K$ is the $\bar{K}\pi$ helicity angle; $\vartheta_3 \equiv \phi$ is the azimuthal angle; and q^2 is the square of the dilepton mass. The q^2 -differential

decay width reads

$$\frac{d\Gamma}{dq^2} = \frac{(3J_{1c} - J_{2c}) + 2(3J_{1s} - J_{2s})}{3}. \quad (C2)$$

It is convenient to define the basis of angular functions and its dual in terms of associated Legendre polynomials $p_l^m(x)$. The index i should thus be interpreted as a multi-index, $i \equiv (l_1, l_2, m)$, where $0 \leq l_1 \leq 2$ and $0 \leq l_2 \leq 2$ denote the total angular momentum in the dilepton and the $K\pi$ system, respectively, and $-2 \leq m \leq 2$ is the third component of either of the angular momenta. We use the same bases of angular functions as given in eq. (B2) and eq. (B3) for the decay $\Lambda_b \rightarrow \Lambda \ell^+ \ell^-$.

In that case, the angular observables correspond to the usual choice of observables via

$$8\pi S_{0,0,0} = 1, \quad 8\pi S_{0,1,0} = \frac{3J_{1i} - J_{2i}}{d\Gamma/dq^2}, \quad 8\pi S_{0,2,0} = \frac{6(J_{1c} - J_{1s}) - 2(J_{2c} - J_{2s})}{3d\Gamma/dq^2}, \quad (C3)$$

and

$$\begin{aligned} 8\pi S_{1,1,-1} &= \frac{6J_{7i}}{d\Gamma/dq^2}, & 8\pi S_{1,2,-1} &= \frac{4\sqrt{3}J_7}{d\Gamma/dq^2}, \\ 8\pi S_{1,0,0} &= \frac{J_{6c} + 2J_{6s}}{d\Gamma/dq^2}, & 8\pi S_{1,1,0} &= 0, & 8\pi S_{1,2,0} &= \frac{2(J_{6c} - J_{6s})}{d\Gamma/dq^2}, \\ 8\pi S_{1,1,+1} &= \frac{6J_{5i}}{d\Gamma/dq^2}, & 8\pi S_{1,2,+1} &= \frac{4\sqrt{3}J_5}{d\Gamma/dq^2}, \end{aligned} \quad (C4)$$

and

$$\begin{aligned} 8\pi S_{2,2,-2} &= \frac{8J_9}{d\Gamma/dq^2}, \\ 8\pi S_{2,1,-1} &= \frac{4\sqrt{3}J_{8i}}{d\Gamma/dq^2}, & 8\pi S_{2,2,-1} &= \frac{8J_8}{d\Gamma/dq^2}, \\ 8\pi S_{2,0,0} &= \frac{4(J_{2c} + 2J_{2s})}{3d\Gamma/dq^2}, & 8\pi S_{2,1,0} &= \frac{4J_{2i}}{d\Gamma/dq^2}, & 8\pi S_{2,2,0} &= \frac{8(J_{2c} - J_{2s})}{3d\Gamma/dq^2}, \\ 8\pi S_{2,1,+1} &= \frac{4\sqrt{3}J_{4i}}{d\Gamma/dq^2}, & 8\pi S_{2,2,+1} &= \frac{8J_4}{d\Gamma/dq^2}, \\ 8\pi S_{2,2,+2} &= \frac{8J_3}{d\Gamma/dq^2}. \end{aligned} \quad (C5)$$

As before, for the purpose of unfolding acceptance effects as laid down in section III B, it is instrumental to know that $f_{0,0,0} \equiv 1$, and that $\max_{\cos\vartheta_1, \cos\vartheta_2, \phi} |f_{l_1, l_2, m}| \leq 1$. The recipe's generating PDFs are therefore $P(x|\{S_i^{(j)}\})$ with

$$S_i^{(j)} = \frac{1}{8\pi} \begin{cases} \delta_{i,(0,0,0)} & j = (0,0,0) \\ \delta_{i,(0,0,0)} + \delta_{i,j} & j \neq (0,0,0) \end{cases} \quad (C6)$$

where also j is now a multi-index representing $j \sim (l_1, l_2, m)$.

To conclude this section, we remind that the angular momentum l_2 , associated with the angle ϑ_2 , is not bounded from above. This has to be considered if partial waves beyond the P-wave are included in the analysis, see e.g. [21]. However, our choice of basis is well suited to these applications with $0 \leq l < \infty$. Note, that the physical range of m is not affected by higher partial waves.

Appendix D: On the Partial-Wave Expansion of Angular Observables

For convenience, we use this appendix to collect there necessary formulae needed in the partial-wave expansion. Let us assume that the angular decomposition has been achieved for some PDF P for all angles except for one

angle ϑ . We now focus on just one of the resulting observables and denote it by $S(\vartheta)$. The dependence on the non-angular variables will be ignored in the following. Suppose S has an expansion in terms of partial waves $l_1, l_2 = 0, 1, 2, \dots \hat{=} \text{S, P, D, } \dots$ of the underlying amplitudes A_1 and A_2 ,

$$S(\vartheta) \equiv F[A_1(\vartheta)A_2^*(\vartheta)] \equiv F\left[\left(\sum_{l_1=0}^{\infty} A_1^{(l_1)} p_{l_1}^{(m_1)}(\cos \vartheta)\right) \left(\sum_{l_2=0}^{\infty} A_2^{*(l_2)} p_{l_2}^{(m_2)}(\cos \vartheta)\right)\right], \quad (\text{D1})$$

where $F \in \{\text{Re}, \text{Im}\}$ denotes taking either the real or the imaginary part. Here $p_l^{(m)}$ denotes an *associated Legendre* polynomial and m_i is the third component of the angular momentum of the amplitude A_i , and we impose $m_1 \geq m_2$.

From the orthogonality of the Legendre polynomials, one immediately finds

$$\int d\cos \vartheta |A_i(\vartheta)|^2 = \sum_{l_i=0}^{\infty} |A_i^{(l_i)}|^2 n_{l_i, m_i} < S_{\text{incl}}, \quad (\text{D2})$$

where S_{incl} is the corresponding observable in the associated inclusive decays, and where we introduce $n_{l,m}$ via the scalar product of two associated Legendre polynomials,

$$\begin{aligned} n_{l,m} \delta_{l,l'} &\equiv \int_{-1}^1 d\cos \vartheta p_l^{(m)}(\cos \vartheta) p_{l'}^{(m)}(\cos \vartheta) \\ &= \frac{2}{(2l+1)} \frac{(l+m)!}{(l-m)!} \delta_{l,l'}. \end{aligned} \quad (\text{D3})$$

The positivity of the amplitudes in eq. (D2) implies that we can estimate the error introduced by cutting off the expansion at some arbitrary angular momentum L . One obtains

$$|A_i^{(l'>L)}|^2 < S_{\text{incl}} - \sum_{l=0}^L |A_i^{(l)}|^2. \quad (\text{D4})$$

Will will show in the following that such a cutoff is compatible with defining a basis of angular observables as coefficients of Legendre polynomials in $\cos \vartheta$. Since this expansion implies a well defined total angular momentum for each observable, one ensures that the observables can in fact be disentangled experimentally.

We decompose S in terms of the associated Legendre polynomials $p_j^{(m)}(\cos \vartheta)$, with total angular momentum j and its third component $m = m_1 + m_2$.

$$S(\vartheta) = \sum_j S_{j,m} p_j^{(m)}(\cos \vartheta). \quad (\text{D5})$$

This parametrization has two merits. First, we can immediately project out the angular observables $S_{j,m}$ by means of eq. (D3):

$$S_{j,m} = \frac{1}{n_{j,m}} \int_{-1}^{+1} d\cos \vartheta S(\vartheta) p_j^{(m)}(\cos \vartheta). \quad (\text{D6})$$

(Here and in the next step we may exchange the integral and the series because each element of the series is a product of polynomials on the compact support $[-1,1]$, and thus each integral is absolutely convergent). Second, we can immediately express $S_{j,m}$ in terms of the partial-wave amplitudes,

$$\begin{aligned} S_{j,m} &= \frac{1}{n_{j,m}} \int_{-1}^{+1} d\cos \vartheta p_j^{(m_1+m_2)}(\cos \vartheta) \sum_{l_1, l_2=0}^{\infty} F\left[A_1^{(l_1)} p_{l_1}^{(m_1)}(\cos \vartheta) A_2^{*(l_2)} p_{l_2}^{(m_2)}(\cos \vartheta)\right] \\ &= \sum_{l_1, l_2=0}^{\infty} F\left[A_1^{(l_1)} A_2^{*(l_2)}\right] \frac{T_{l_1, l_2, j}^{(m_1, m_2)}}{n_{j,m}}, \quad \text{with } m = m_1 + m_2. \end{aligned} \quad (\text{D7})$$

In the last step, we use Gaunt's formula [26] to integrate a triple product of associated Legendre polynomials,

$$\begin{aligned}
T_{l_1, l_2, j}^{(m_1, m_2)} &= \int_{-1}^{+1} d \cos \vartheta p_j^{(m_1+m_2)}(\cos \vartheta) p_{l_1}^{(m_1)}(\cos \vartheta) p_{l_2}^{(m_2)}(\cos \vartheta) \\
&= (-1)^{s-l_1-m_2} \frac{2(l_1+m_1)!(l_2+m_2)!(2s-2l_2)!s!}{(l_1-m_1)!(s-j)!(s-l_1)!(s-l_2)!(2s+1)!} \\
&\times \sum_{t=p}^q (-1)^t \frac{(j+m+t)!(l_1+l_2-m-t)!}{t!(j-m-t)!(l_1-l_2+m+t)!(l_2-m_2-t)!},
\end{aligned} \tag{D8}$$

where

$$\begin{aligned}
m &= m_1 + m_2, & m_1 &\geq m_2, \\
j, l_1, l_2 &\geq 0, & m, m_1, m_2 &\geq 0,
\end{aligned} \tag{D9}$$

and

$$\begin{aligned}
s &\equiv \frac{j + l_1 + l_2}{2}, \\
p &\equiv \max(0, l_2 - l_1 - m), \\
q &\equiv \min(l_1 + l_2 - m, j - m, l_2 - m_2).
\end{aligned} \tag{D10}$$

The necessary conditions for $T \neq 0$ are

$$s \in \mathbb{N} \quad \wedge \quad l_1 - l_2 \leq l \leq l_1 + l_2, \tag{D11}$$

The latter condition is well known from the addition rules of angular momenta. Note, however, that the sum in eq. (D1) goes to infinitely high angular momenta l_1 and l_2 . As a consequence of this and of eq. (D11), the angular observables $S_{j,m}$ consist of sums with infinitely many terms. It is then up to theoretical analyses to estimate or calculate the impact of the neglected partial waves, e.g. as outlined above.

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